

RmassBankGUI Tutorial

0. Prerequisites

- Install the RMassBank, XCMS, and CAMERA libraries (Supplied by the workshop staff)
- Install the tcltk package from CRAN
`install.packages("tcltk")`
- Create an empty folder in which you want to save all your projects

1. Installing RMassBankGUI

To install RMassBankGUI directly from its github repository, use the devtools-package. If the devtools-package isn't installed yet, you can install it from CRAN by simply typing

```
install.packages("devtools")
```

To install RMassBankGUI type

```
library(devtools)  
install_github("ermueller/RMassBankGUI")
```

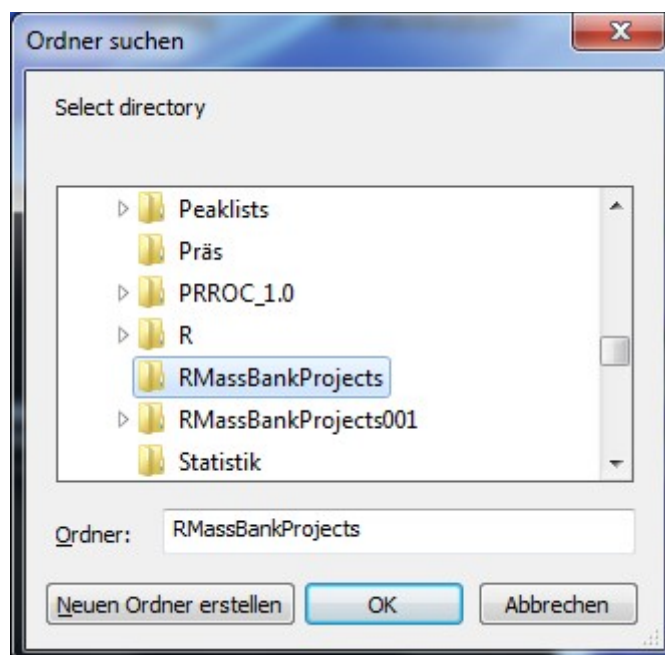
2.1 Using RmassBankGUI

To create records using RMassBankGUI the GUI-package needs to be loaded in R by typing
`library(RMassBankGUI)`

To start the GUI type
`startRMBGUI()`

Now the GUI should start and prompt you to select a folder to save your projects. Choose your previously created folder and press OK.

After this the project manager should open. If you accidentally chose the wrong folder, press the



“Change folder” button to change your project folder. Since there currently are no projects, a new one has to be created. In the window opening now you can fill out parameters for the project you want to create.

Project Specifications

Name of Project:	
Author(s) of the project:	
Copyright:	Copyright (C) XXX
Publication:	
License:	
Instrument:	
Instrument type:	
Confidence comment:	standard compound
Compound class:	N/A; Environmental Standard
Internal ID:	INTERNAL_ID
Entry prefix:	XX
MS Type:	MS2
Ionization:	ESI
FLOW_GRADIENT:	90/10 at 0 min, 50/50 at 4 min, 5/95 a
FLOW_RATE:	200 uL/min
SOLVENT A:	water with 0.1% formic acid
SOLVENT B:	water with 0.1% formic acid
COLUMN_NAME:	XBridge C18 3.5um, 2.1x50mm, Water

Buttons: Import settings for project, Create project with these parameters

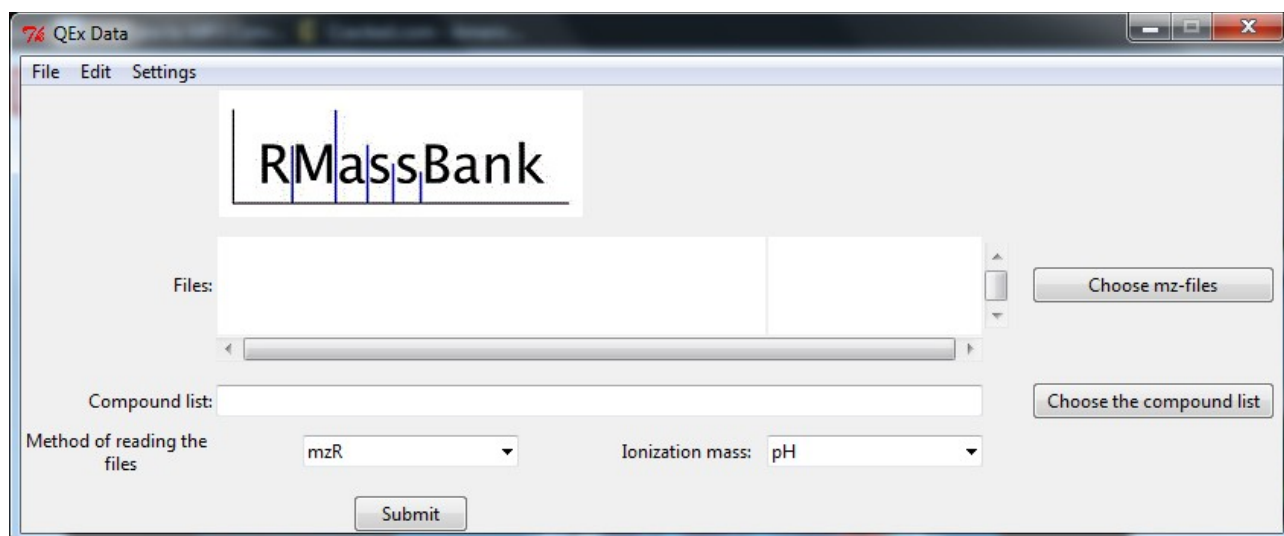
The fields marked with red labels are mandatory, while all others are optional. After everything is filled out, you can create the project with these parameters and choose it in the project manager.

RMassBank GUI Start Window

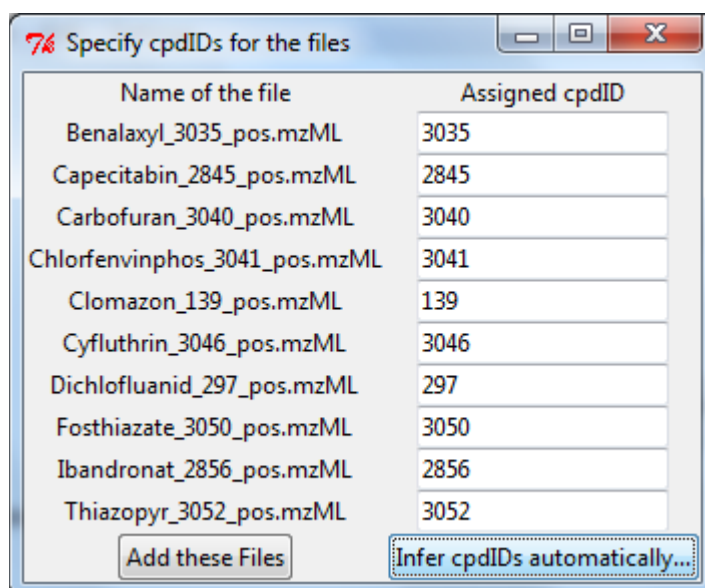
QEx Data

Buttons: Create new project, Choose selected project

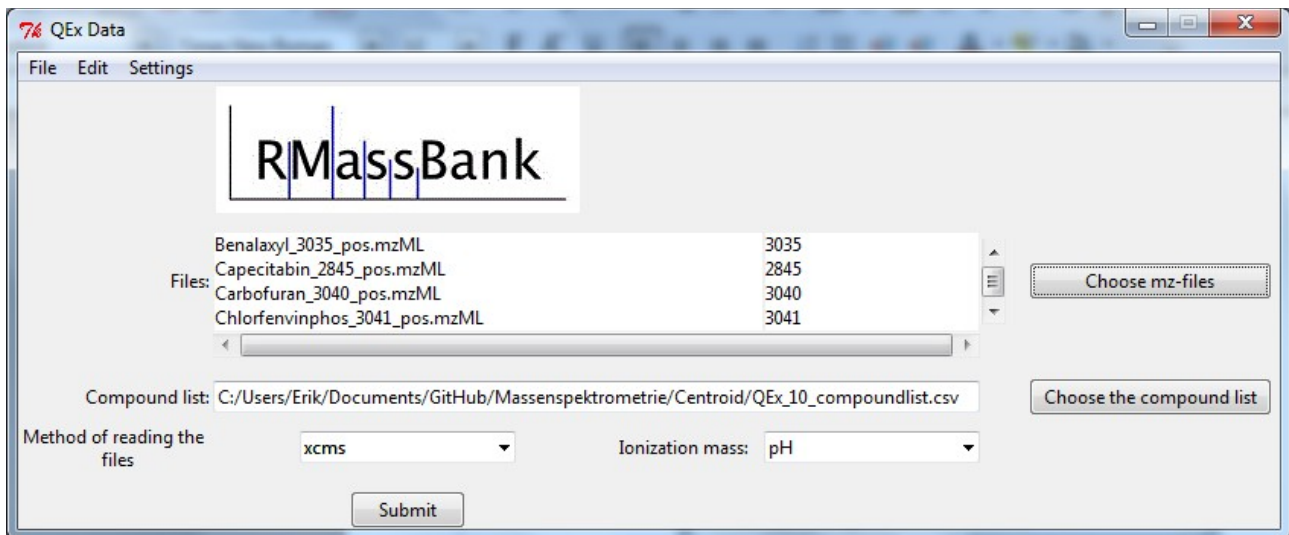
After choosing the project, the main GUI window opens.



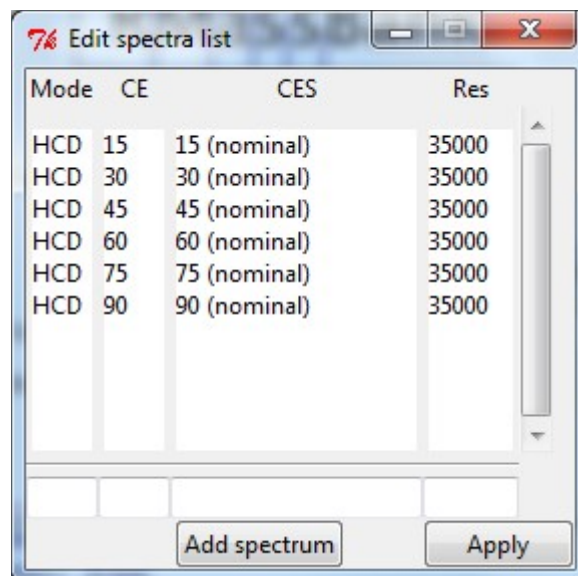
You can now choose the files by clicking the “Choose mz-files”-Button. This will open a file browser and subsequently after choosing the files will open a window where you can assign cpdIDs to the proper files manually or you can try to infer them automatically. (This only works when the files are named after RMassBank naming convention) Choose the QEx-files and infer the cpdIDs, then click “Add these Files”.



With the files added you now have to choose the compound list by using the “Choose the compound list” button (or by manually typing in the file path to the compound list)
At this point, choose the compound list for the QEx-Data



At this point you need to edit the spectra list by going to the settings menu and choosing “Edit spectra list” at which point a window for editing the spectra list will open. The four fields at the bottom correspond to the column they are in and upon pressing the “Add spectrum” button the values from these entries will be added to the spectra list. After filling out the spectra list as shown in the picture press “Apply”.



To generate records choose your preferred method of reading files and leave the ionization parameter at “pH”.

After setting everything up go to File → Save, to save the current state of the project.

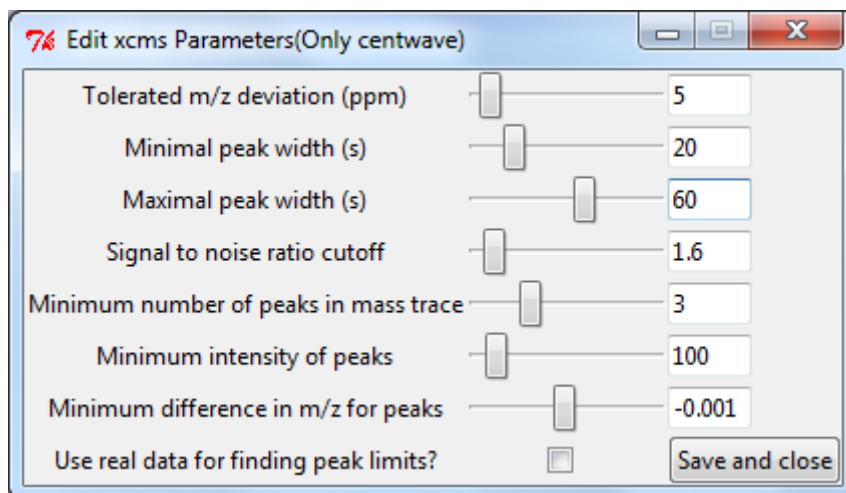
After this, click submit and you can follow the process of the record generation in the R window. (A graphical progressbar is still in testing phase)

The records will be in your R working directory for evaluation.

2.2 Advanced settings

2.1 XCMS Settings

The advanced settings for record generation have been implemented for XCMS. To open the advanced settings for XCMS click



Settings → Edit xcms parameters

The parameters edited here are used for the centwave-method of XCMS (See also: XCMS documentation) It is currently strongly advised to use the XCMS readmethod only with centroid data.

2.2 Changing Project parameters

If you want to change the project parameters choose

Settings → Edit Project settings

and a window very much alike the window to create projects will pop up, enabling you to change the annotations of the project.